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# Accurate modeling and reconstruction of three-dimensional percolating filamentary microstructures from two-dimensional micrographs via dilation-erosion method

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ABSTRACT

Heterogeneous materials are ubiquitous in nature and synthetic situations and have a wide range of important engineering applications. Accurate modeling and reconstructing three-dimensional (3D) microstructure of topologically complex materials from limited morphological information such as a two-dimensional (2D) micrograph is crucial to the assessment and prediction of effective material properties and performance under extreme conditions. Here, we extend a recently developed dilation–erosion method and employ the Yeong–Torquato stochastic reconstruction procedure to model and generate 3D austenitic–ferritic cast duplex stainless steel microstructure containing percolating filamentary ferrite phase from 2D optical micrographs of the material sample. Specifically, the ferrite phase is dilated to produce a modified target 2D microstructure and the resulting 3D reconstruction is eroded to recover the percolating ferrite filaments. The dilation–erosion reconstruction is compared with the actual 3D microstructure, obtained from serial sectioning (polishing), as well as the standard stochastic reconstructions incorporating topological connectedness information. The fact that the former can achieve the same level of accuracy as the latter suggests that the dilation–erosion procedure is tantamount to incorporating appreciably more topological and geometrical information into the reconstruction while being much more computationally efficient.



## 1. Introduction

Heterogeneous materials such as composites, alloys, granular materials and porous media abound in nature and in engineering applications. Applications of heterogeneous materials in civil, industrial and aerospace engineering require accurate assessments and predictions of the effective material properties and their performance under extreme conditions, which in turn rely on the accurate knowledge of the complex material microstructures. In the past few decades, a quantitative under-

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standing of the microstructure and structure–property relation of heterogeneous materials has begun to emerge, mainly due to the development of advanced experimental and computational material microstructure characterization techniques [1–3]. Specifically, advanced imaging techniques such as X-ray tomographic microscopy [4–6], which eliminates destructive cross-sectioning and allows for superior resolution and image quality with minimal sample preparation [7,8], have been widely used to obtain high-resolution three-dimensional (3D) microstructure for a wide range of heterogeneous materials, including Sn-rich alloys [9], powder metallurgy steels [10], metal matrix composites [11–15], and lightweight alloys [16–20]. On the theory side, a zoology of statistical microstructure descriptors has been presented and derived from rigorous structure–property analysis [1,2]. For example, the canonical $n$-point correlation function $H_n$ [2], the integrals of which are involved in various rigorous bounds [21] and contrast expansions [22,23] of effective material properties, gives the probability of finding a specific $n$-point configuration in the phase of interest. A variety of non-canonical descriptors providing topological connectedness information [24–26] and interface information [27] have also been devised and applied to study a wide spectrum of materials.

Despite of rapid advances of non-destructive 3D imaging techniques, there are still material systems for which only 2D images are available. For example, in certain alloys the contrast between the absorption rates of probing rays associated with different phases is too weak to resolve the individual phases. In such situations, usually the only available structural data obtained from non-destructive means are 2D electron micrographs or optical images of the sample surfaces, which does not contain topological connectedness information of the material phases [2]. Although serial sectioning can be employed to obtain full 3D microstructure, this procedure is very tedious and will completely destroy the material sample. Therefore, it is highly desirable to render realistic virtual 3D microstructures that faithfully present the limited morphological information contained in the available 2D data sets, albeit with 3D experimental verification.

Over the past two decades, a variety of microstructure reconstruction methods from limited structural information have been developed, including the Gaussian random field method [28], stochastic reconstruction procedure [29,30], phase recovery method [31], multi-point reconstruction method [32], and raster-path method [33]. The Gaussian random field method [28] was originally devised to reconstruct realizations of statistically homogeneous and isotropic random media from the associated two-point correlation functions. Specifically, a field-field correlation function is constructed based on the given two-point correlation function $S_2$ (see definition in Section. 2). A Gaussian random field is then generated using the field-field correlation function, whose level-cut results in a binary microstructure associated the target two-point function. Although a wide class of microstructures can be obtained using this method, the morphological information used for reconstruction is limited to the two-point correlation functions [28]. The phase recovery method enables one to take into account the full vector information contained in the two-point statistics associated with the material, and thus allows the reconstructions of complex anisotropic microstructure and polycrystalline materials [31]. This method proceeds by iteratively solving for the phase information that is lost when representing the microstructure using the vector two-point correlation functions. Once such phase information is successfully recovered, the microstructure can be directly obtained via fast Fourier transform.

The multi-point reconstruction method was originally developed for the reconstruction of porous geomaterials from 2D images [32]. Instead of using two-point statistics associated with the entire 2D microstructure, this method incorporates all $n$-point statistics within a smaller window containing a portion of the microstructure. The window size is determined by the correlation length of the material. A sequential addition method is then employed to put down voxels in an initially empty reconstruction domain based on the $n$-point statistics to generate a 3D microstructure. Although more accurate reconstructions can be obtained due to the additional morphological information contained in the multi-point statistics, it is difficult to efficiently store, represent and retrieve the $n$-point statistics even for a very small window. Recently, a raster-path method is devised which allows one to employ the multi-point statistics in a much more efficient way [33]. Specifically, instead of extracting the statistics from the 2D microstructure, a cross-correlation function is introduced to directly compare a reconstructed portion of the material to the target 2D image. Only the reconstructed portions that sufficiently well match a portion in the target microstructure will be accepted and inserted into an initially empty reconstruction domain along a 1D raster path [33].

The stochastic reconstruction procedure [29,30] (also referred to as Yeong–Torquato procedure in literature) enables one to incorporate an arbitrary number of correlation functions of any types into the reconstructions. Specifically, a random initial microstructure is evolved using simulated annealing procedure such that the set of correlation functions sampled from the reconstructed microstructure match the corresponding set of target statistics up to a prescribed small tolerance (see Section. 3 for algorithmic details). This reconstruction procedure is very flexible and versatile, however, due to its stochastic nature a large number of intermediate microstructures need to be generated and analyzed, which makes it computationally intensive. Several different implementations of the Y–T procedure have been devised to improve efficiency [34–36], preserve isotropy [37–39] or handle anisotropic materials [40]. In particular, a dilation–erosion (DE) method based on the Y–T procedure has recently been proposed by Zachary and Torquato to improve the accuracy of the reconstructions of topologically complex microstructures [41]. The DE method (discussed in detail in Section. 3) has been applied to successfully reconstruct 2D model microstructures including multiply connected “donut” media and random distributions of micro-cracks [41].

In this paper, we will extend the dilation–erosion procedure devised by Zachary and Torquato [41] for 2D random textures to accurately model and reconstruct 3D filamentary microstructures from limited morphological information (e.g., certain spatial correlation functions associated with the filamentary phase) available in 2D images of the material. We will focus on austenitic–ferritic cast duplex stainless steels for which the 2D optical micrographs of the sample surfaces (see Fig. 1) will be used as the input for the reconstruction. As shown in Fig. 1, the filamentary structures correspond to the ferrite phase which percolates in three dimensions. Such percolating filamentary